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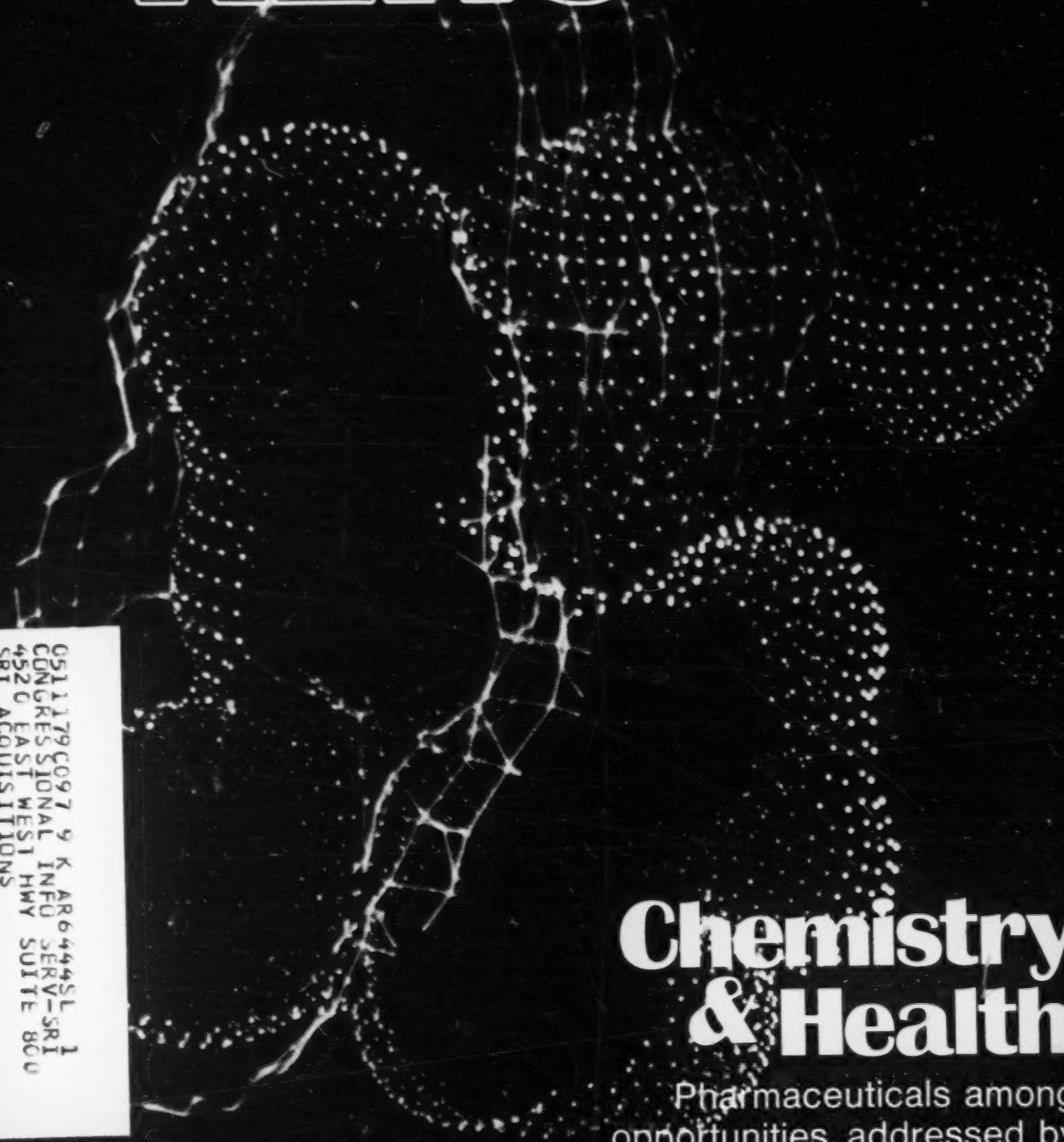
NOVEMBER 3, 1986

CHEMICAL & ENGINEERING

NEWS



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Chemistry & Health

Pharmaceuticals among opportunities addressed by CHEMRAWN V Page 7

CHEMICAL & ENGINEERING
NEWS
Volume 64, Number 44
CENEAR 64 (44) 1–60
ISSN 0009-2347
NOVEMBER 3, 1986

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Cover: Computer-generated images help drug researchers visualize complex structures; close resemblance in geometry and volume of D-alanyl-D-alanine dipeptide (green and magenta structure) and benzyl-penicillin (blue structure and dot surface) indicates that the two may bind to transpeptidase inhibitors. Photo courtesy of University of Bern and Evans & Sutherland

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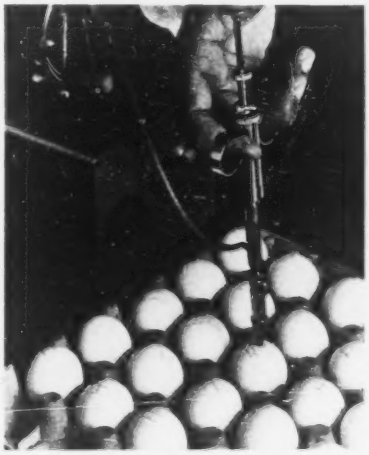

News Focus

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Propylene Use in Western Europe Showing Steady Gains

Its use to make chemicals, currently growing nearly 3% annually, is increasing faster than ethylene's, is expected to hit 16.5 billion lb in 1990

Dermot A. O'Sullivan, C&EN London

Propylene is something of an orphan in the petrochemical world. Although it is key to a wide range of derivatives, few suppliers set out to make it as their prime product. "Rather, it is everybody's coproduct, or even by-product," Howard E. Browning, marketing manager for olefins, aromatics and bulk petrol at Imperial Chemical Industries' petrochemicals and plastics division, told delegates to the European Chemical Market Research Association meeting in Antwerp.

Although propylene demand is on the rise, mainly because of increasing use of polypropylene, supply is largely dependent on output from ethylene-making crackers, as well as the economics of oil refinery operations. So price fluctuates widely as availability is "long" or "short."

West European production of propylene last year amounted to about 18.7 billion lb. Some 72%, or 13.4 billion lb, came from crackers, and the remainder from oil refineries. Discounting the nearly 3.1 billion lb used by the refiners themselves, 15.6 billion lb was made available to the chemical industry. An additional 550 million lb or so was imported—mainly from Eastern Europe, Latin America, and the U.S., bringing the total for making chemicals to 16.2 billion lb.

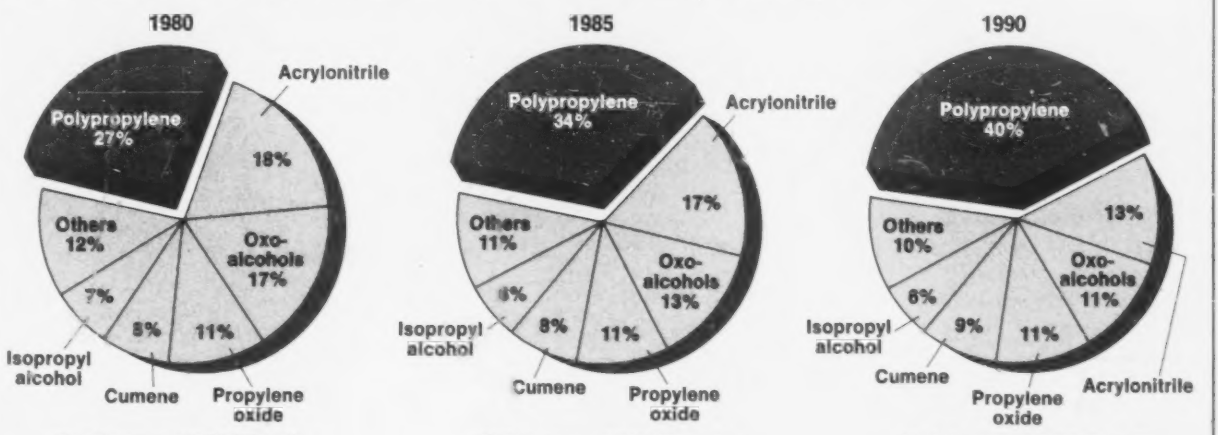
On the demand side, more than 15.8 billion lb went into chemicals in 1985. Polypropylene output absorbed the largest slice (34%), followed by acrylonitrile, oxo-alcohols, propylene oxide, cumene, and isopropyl alcohol, in addition to a variety of chemical operations.

"Polypropylene is the prime engine for propylene growth in Western Europe," Browning observes. "It has been following a classic product life cycle curve ever since its commercialization in the late 1950s, and is still very much in the growth phase. Not only is this true of the product as a whole, but its individual end-use applications are widespread, and all are growing strongly."

He expects West European demand for the polymer to reach 6.6 billion lb in 1990, just about double the nearly 3.4 billion lb consumed in 1980, and representing a 7%-a-year growth over the decade. Moreover, he thinks it likely that production of the polymer will absorb 40% of the propylene used by the European chemical industry in 1990, in contrast to the 27% level in 1980.

As for acrylonitrile and the oxo-alcohols, the markets themselves are reasonably stable. However, increasing efficiency in the use of propylene for their production probably will lead to a decline in the actual

Polypropylene takes growing share of Western Europe's propylene



Source: Imperial Chemical Industries

C&EN staff photo

Browning: everybody's coproduct

amount of the olefin that goes into them. And although Browning anticipates some growth ahead for propylene oxide in making polyurethanes and surfactants, and for cumene as the precursor of phenol, he points out that these "account for a relatively small percentage of the propylene demand." Isopropyl alcohol use likely will remain flat for the next several years.

Overall, he expects that the West European chemical industry will require about 16.5 billion lb of propylene in 1990 compared with nearly 12.5 billion lb in 1980. That would represent a 2.9% annual growth in use—relatively high when compared with the anticipated yearly growth rate of 1.2% predicted for ethylene, and 1.6% for industrial output as a whole, during the 10-year period.

Browning sees a gap widening between the quantity of propylene coproduced in Western Europe's crackers and need for the olefin by the chemical industry there. "The prime purpose of steam crackers," as he points out, "is to make ethylene." The "quite good" capacity utilization of the cracker population likely will result in the crackers' declining ability to keep pace with increasing propylene demand, he reasons.

The type of feedstock used and the severity of the cracking operations also have a significant effect on the relative amount of propylene produced. At one time, naphtha was used almost exclusively in crackers throughout Europe. This feedstock gives rise to about a pound of propylene for every 2 lb of ethylene. But there is a trend to build flexibility into the crackers to allow use of such "lighter" feedstocks as liquefied petroleum gas and ethane, with a resulting drop in propylene output. Indeed, in the case of ethane, the level of propylene made is negligible.

Not only is a cracker's propylene output dependent on the type of feedstock used, but the conditions of operation is a factor. High temperatures favor ethylene formation; at lower temperatures, relatively more propylene is produced. Reducing the severity of the cracking could increase the amount of propylene available to West European chemical makers by up to 3.3 billion lb a year, Browning estimates. "In practice, however, some operators will not want to change," he believes.

European petrochemical companies in the market for propylene are benefiting from the move that is gaining momentum to reduce the amount of lead additives in gasoline for environmental reasons. As recently as two years ago, practically all the gasoline used throughout Western Europe contained 0.4 g per L of lead, mostly as tetraethyllead antiknock compound. Now, several countries have taken steps to reduce the lead in their gasoline pool. By 1990, only some 20% of West European gasoline is expected to remain leaded at the 0.4 g-per-L level. In 40%, it will be down to 0.15 g per L. The remaining 40% or so will be lead-free.

"To accommodate the removal of lead, the 'clear octane' value of the gasoline pool [the inherent octane rating of a fuel before blending in additives] must rise," he observes. "Fluidized catalytic crackers (FCCs) are playing an increasing role in helping refiners meet this demand."

One outcome of the move to fluid catalytic cracking is an increase in the relative abundance of propylene in the refinery streams. "The more FCCs become economically viable, the harder they will get driven to raise the octane number, and the more propylene will result," Browning says. "Additionally, the newer catalysts being employed in the FCCs favor propylene yield. The net effect of all this is that more propylene is being produced in European refineries, and there now is a steady increase in the amount being purified for chemical use."

Propylene demand isn't the prime driving force either of steam cracker operators or refinery managers. But because demand for propylene is growing faster than that for ethylene, it isn't surprising that on a long-term basis the ratio between propylene and ethylene prices is steadily rising, he reasons.

"From a level of around 40% of the ethylene price in 1970, propylene now commands a price of about 80% that of ethylene." Although this trend is a fairly steady transition over the past 15 years, the price relationship can undergo wide swings depending on such factors as the degree of demand, the amount of stocks on hand, oil and gas prices, and the like. □

Most propylene uses in Western Europe are growing

Millions of lb	1980	1985	1988[a]	1990[a]	Average annual growth 1980–85	Average annual growth 1985–90
Polypropylene	3,366	5,390	5,786	6,600	9.9%	4.1%
Acrylonitrile	2,200	2,684	2,552	2,200	4.1	−3.9
Oxo-alcohols	2,178	1,980	1,958	1,826	−1.9	−1.6
Propylene oxide	1,386	1,694	1,628	1,738	4.1	0.5
Cumene	1,012	1,298	1,210	1,408	5.1	1.6
Isopropyl alcohol	858	1,012	1,012	1,034	3.4	0.4
Others	1,452	1,694	1,650	1,716	3.1	0.3
TOTAL	12,452	15,752	15,796	16,522	4.8%	1.0%

a Estimates. Source: Imperial Chemical Industries

Congress Approves 8% Increase for Major R&D Funding Agencies

Appropriation bill sets higher funding levels for most federal R&D agencies in fiscal 1987, with NASA and NIH scoring the biggest gains

Janice R. Long, C&EN Washington

Perhaps the most important legislative action taken during the last chaotic days before final adjournment of the 99th Congress was passage of H.J. Res. 738, which rolled into one huge bill the 13 regular appropriation bills that provide funding for all the government departments and agencies in fiscal 1987. Until Congress cleared that measure on Oct. 17, more than two weeks after the beginning of fiscal 1987, none of the federal R&D agencies knew how much money they actually would be able to spend. For some of those agencies, the continuing resolution contained more money for them than was approved earlier by either the House or the Senate. For others, the funding approved was lower.

Most of the agencies will receive more R&D funding this fiscal year than in fiscal 1986, with the total budget for major R&D agencies up 8% to $53.4 billion. The two biggest gains are for the National Aeronautics & Space Administration, whose R&D budget is up 19% to $3.13 billion, and the National Institutes of Health, whose R&D budget is up 20% to about $6.0 billion. The Administration had wanted to cut NIH's total budget 9%, but Congress once again performed its annual rescue operation, approving more than either the House or the Senate had done in their appropriation bills. Within NIH's budget, funding for the National Institute of Allergy & Infectious Diseases is up an astonishing 65% to $546 million, primarily owing to its part of the $248 million included in the bill for research on acquired immune deficiency syndrome (AIDS).

Overall, Congress expects the budget total for NIH to support at least 6100 new and competing research grants—a number that the Office of Management & Budget has been trying to reduce in recent years—and at least 10,500 trainees.

The Department of Defense's R&D budget, up 8% to $37 billion, didn't fare so well percentagewise as those for NASA and NIH. Nor did it match the 22% increase to $42 billion that the Administration was seeking. Nonetheless, it remains by far the largest single component of federal R&D funding. However, only 8% of that $37 billion, or $3 billion, will be spent on DOD's technology base—that is, basic research activities, which are funded at a level only 2% higher than last year and which provide funds for DOD-sponsored university research. But funding for another DOD program that supports university-based research, the Strategic Defense Initiative, is up 18% to $3.2 billion. The Administration had requested a 77% increase to $4.8 billion.

Given DOD's increasing investment in university-based research, Congress has requested a report that explains in detail DOD's current peer-review process in a step-by-step fashion. It must describe participants in this process and how they are chosen, and analyze the potential for expanding the research base into geographic areas that now receive little defense-related university funding. The resolution also directs DOD to develop a five-year plan providing for sustained real growth in both the University Research Initiative and the armed services' university research programs.

The resolution also limits the testing of antisatellite weapons in space

In its final days, 99th Congress passes several major bills

The 99th Congress has passed into history. Its final days were chaotic with bills flying back and forth between the House and Senate during sessions that lasted far into the night. Out of that chaos emerged important pieces of legislation in addition to the large appropriations bill. These include:

- An omnibus antidrug bill that mandates stiff penalties for manufacture, distribution, or possession of so-called "designer drugs."
- An immigration reform bill that does not, as earlier versions did, impose new requirements on foreign students.
- A bill allowing exports of drugs that have not been approved for use in the U.S.
- Amendments to the Clean Water Act that set strict criteria and timetables for limiting discharges of toxic pollutants into waterways.
- An $8.5 billion five-year reauthorization of the abandoned hazardous waste site cleanup program called Superfund.
- Legislation allowing those seeking liability insurance to establish on an interstate basis either a "risk retention group" to self-insure, or a group to purchase such insurance cooperatively.
- Fiscal 1987 authorization bills for the Department of Defense, National Aeronautics & Space Administration, National Bureau of Standards, and Patent & Trademark Office.

Funding for major R&D agencies rises about $4 billion

$ Millions	1987 Congressional appropriation	1987 Administration request	1986	% change 1986–87
Defense	**$36,622.1**	**$41,740.3**	**$34,057.3**	**8%**
Tactical programs	11,422.3	12,671.4	10,546.7	8
Strategic programs	8,352.9	9,429.5	7,796.9	7
Intelligence and communications	4,996.8	5,066.8	4,504.2	11
Advanced technology development	4,746.9	6,574.7	4,170.8	14
Defensewide mission support	3,766.6	4,413.0	3,780.9	—
Technology base	3,336.6	3,584.9	3,257.8	2
NIH	**5,939.7**	**4,833.8**	**4,983.1**	**20**
Cancer	1,402.8	1,158.1	1,176.8	19
Heart, Lung & Blood	930.1	785.7	810.8	18
General Medical Sciences	570.9	471.5	492.4	16
Allergy & Infectious Diseases	545.5	340.8	330.5	65
Diabetes & Digestive and Kidney Diseases	511.1	418.9	433.5	18
Neurological & Communicative	490.2	399.3	413.0	19
Child Health & Human Development	366.8	309.1	307.7	19
Eye	216.6	179.2	186.5	16
Environmental Health Sciences	209.3	188.0	188.9	11
Aging	176.9	145.8	142.6	24
Arthritis & Musculoskeletal and Skin Diseases	138.7	106.7	110.7	25
Dental research	117.9	96.5	98.1	20
Research resources	322.9	234.2	290.7	11
Energy	**3,903.1**	**3,844.2**	**3,824.0**	**2**
Energy supply R&D	**1,644.4**	**1,677.0**	**1,658.1**	**− 1**
Supporting research and technical analysis	524.0	618.6	487.7	7
Fusion	345.5	333.0	365.5	− 6
Nuclear R&D	327.5	330.9	375.7	−13
Environment	273.9	258.1	228.6	20
Solar	124.2	72.3	144.6	−14
Other	49.3	34.1	56.0	−12
Weapons R&D	**1,103.1**	**1,239.9**	**1,015.4**	**9**
General science and research	**708.4**	**773.4**	**655.9**	**8**
Fossil R&D	**295.5**	**82.8**	**311.0**	**− 5**
Conservation R&D	**151.7**	**71.1**	**183.6**	**−17**
NASA R&D	**3,127.7**	**3,032.1**	**2,638.3**	**19**
NSF	**1,622.1**	**1,685.0**	**1,483.8**	**9**
Research and related activities	1,406.1	1,479.0	1,294.1	9
Antarctic programs	117.0	117.0	110.0	6
Science education	99.0	89.0	84.7	17
Commerce	**1,160.6**	**960.4**	**1,215.9**	**− 5**
NOAA	1,038.6	836.5	1,097.2	− 5
NBS	122.0	123.0	118.7	3
USDA	**966.6**	**870.9**	**885.7**	**9**
Agricultural Research Service	537.1	513.0	484.1	11
Cooperative State Research Service	300.6	246.4	276.1	9
Forest Service research	128.9	111.5	125.5	3
EPA R&D	**303.5**	**295.2**	**324.6**	**− 7**
TOTAL	**$53,405.4**	**$57,261.9**	**$49,417.7**	**8%**

Note: All figures are estimates. **Source:** Congressional budget documents

and the production of the Bigeye binary chemical bomb. No test of antisatellite weapons can be carried out until the President certifies that the Soviet Union has conducted, after the date the resolution was signed, a test of a dedicated antisatellite weapon against an object in space. The resolution also states that no funds may be obligated for procurement or assembly of the Bigeye bomb before Oct. 1, 1987.

The National Science Foundation was one agency that was hoping for more from the continuing resolution than it got. NSF wanted the resolution to go along with the Senate reversal of the House's decision to cut $136 million from NSF's total budget request and $146 million from the research and related-activities request. NSF had warned that if the House action was allowed to stand, it would result in the loss of some 1000 grants, eliminating support for about 1500 scientists and engineers. The continuing resolution, however, splits the difference between the House and Senate positions, giving NSF a 9% increase in its total budget to $1.6 billion and also a 9% increase, not the requested 14%, in its research and related-activities budget to $1.4 billion.

The funding measure also does not fully restore the $5 million the House cut from the $101 million budget request for the Department of Energy's chemical sciences program. Final funding for that program is set at just over $98 million, a 6% increase over fiscal 1986 funding levels. Funding for DOE's materials science program is set at $235 million, 25% over fiscal 1986 and 20% over the budget request, and includes $4 million for the National Center for Chemical Research. DOE's overall R&D budget is up a slight 2% to $3.9 billion.

Among other funding decisions are an 11% increase to $537 million for the Agricultural Research Service and a 3% increase to $122 million for the National Bureau of Standards. However, the budget for the National Oceanic & Atmospheric Administration's research activities is down 5% to $1 billion, and the Environmental Protection Agency's R&D budget is down 7% to $304 million. □

Concerns About World Oil Problems Are Growing

Institute of Gas Technology conference addresses negative impacts of oil price drop and its potential for causing future oil crises

Joseph Haggin, C&EN Chicago

The recent drop in crude oil prices has a down side that many people view as a crisis. Producing countries around the world have been hurt. And in the U.S., the price decline has had a severe economic impact on producing states and on the industry, while the country has increased its reliance on imports. Dealing effectively with the situation will require concerted government action, industry planning, honing national objectives, and international cooperation.

A growing consensus in the U.S. among those most directly affected, including the chemical and petrochemical industries, suggests that preventive measures must be taken soon to avoid panics such as those of 1973 and 1979. In the longer term, the course and character of chemical technology related to energy inevitably will be altered by the measures chosen. But steps taken now could allow that course and character to be determined by users rather than having them dictated from abroad.

That's the situation addressed last month at a conference on "Confronting the Crisis in World Oil" in Houston. The title is the general topic of a new series of symposia sponsored by the Institute of Gas Technology (IGT) and begun with the meeting in Houston.

A common theme in formal and informal discussions at the meeting was that the Organization of Petroleum Exporting Countries may have done itself in with its activities during the past decade. OPEC may possibly display its former solidarity again, but even if it does, the nature of the oil business has changed permanently. Substitution of other fuels for oil, the emergence of C_1 chemistry as an industrial sector, conservation, and growing world reliance on nuclear power leave little doubt that the industrial countries will take pains to avoid another bout of market manipulations by OPEC like those of the 1970s.

The U.S. has been especially hard hit by recent oil-related events. Domestic production has suffered considerably in recent months, and it's feared that additions to reserves will not keep pace in the future because of the demise of the domestic drilling industry. Solutions to that situation depend in large part on the policies of the U.S. government, which, according to some in the oil industry, doesn't always pay enough attention to domestic problems.

The State Department, not surprisingly, considers the greatest problem in the oil business to be OPEC. Marion V. Creekmore, the department's deputy assistant secretary for Near Eastern and South Asian affairs, says the U.S. approach to OPEC has been consistent for a long time. The U.S. government believes, he says, that market forces, and not OPEC producers, should control oil markets and determine prices. The U.S. opposes OPEC and other cartels because they restrain trade.

As Creekmore notes, market forces began to be felt after 1980, despite the action of the cartel. One of the major results was a sharp increase in non-OPEC oil production. OPEC attempted to maintain high prices using production quotas, but revenue squeezes wouldn't permit output to be cut for very long. Saudi Arabia eventually abandoned its role as swing producer, and prices started to drop. OPEC is now trying to regroup and re-establish itself.

The distinction between radical and moderate states in the Persian Gulf region was repeatedly emphasized by Creekmore, who notes that the Gulf Cooperation Council (Saudi Arabia, Kuwait, Oman, the United Arab Emirates, Bahrain, and Qatar) is working toward economic and military integration. The U.S. supports these efforts, he says, and believes that a strong council will increase Middle East stability. That could be of crucial importance if the Iran-Iraq War is settled in favor of Iran in the next few months, as some believe it will be.

Another State Department official, Daniel P. Serwer, director of energy consumer country affairs, outlined the U.S. energy-policy response to falling oil prices. The changes were, he said, strictly responses to market pressures designed to remove "impediments to energy production." The lower oil prices have reduced OPEC's room for maneuvering and, generally, im-

U.S. imports of crude oil increase from last year's level

Thousands of barrels per day	First six months 1985	1986	Change
Field production	9,010	8,872	−138
Imports	2,988	3,600	612
Refinery inputs	11,729	12,497	768
Field production as % of refinery inputs	77%	71%	−6%
Imports as % of refinery inputs	25%	29%	4%

proved the trade picture for most importers. This stimulated economic growth and could be particularly beneficial for countries such as Japan, West Germany, and Italy, where economic growth could be as much as 1% higher than for other members of the Organization for Economic Cooperation & Development (essentially the noncommunist, industrialized countries).

Things aren't quite so rosy in the U.S. Serwer notes that, contrary to expectations, low prices have had a pronounced negative effect on U.S. oil companies, even though the total economy may have benefited. The U.S. is still the world's second largest oil producer, and the economic problems are most severe in the producing states of Texas, Alaska, Oklahoma, and Louisiana. The U.S. is also the largest importer of oil. It cannot let lower prices reverse the positive effects of conservation, substitution, and indigenous production, or energy security will be reduced, Serwer points out. The State Department does not expect this to happen, he says.

However, the government's efforts to ensure energy security have been criticized. One of the most controversial issues has been oil import fees. The Reagan Administration has rejected such import fees on the grounds that they fall heaviest on low-income consumers, erode competitiveness, and cause more problems for heavily indebted exporting countries. The Administration is also accelerating the completion of the strategic petroleum reserve and encouraging allies to likewise build up reserves. But much of the reaction to what the Administration has done to counter the effects of falling prices can be summed up in the statement that it is too little and too late.

The extent of changes in the nature of the oil business was pointed out at the conference by Charles L. Campbell, retired senior vice president of Gulf Oil Corp. He noted that until 1975, more than 80% of the world's oil reserves were in the hands of eight international companies. In 1980, these same companies owned less than 10% of the reserves. In the same period, OPEC gained and then lost control of oil pricing. Campbell maintains that price stability as once administered by the Texas Railroad Commission and the major international oil companies is no longer feasible. No entity now has either the discipline or the appropriate interests to regulate production.

Present excess world production capacity, Campbell explained, operates at low cash costs, and that makes it difficult to justify any new energy projects strictly on the basis of economics. Investment decisions will be made to purchase reserves, existing refineries, and existing market assets rather than to build new facilities or expend risk capital on frontier exploration. So far, the changes in the oil industry have been the result of political or military action, and that pattern is likely to continue, with more nations involved in the total struggle for dominance.

The key historical fact, Campbell says, is that oil is now a commodity. Prices will continue to cycle rapidly with random volatility. Business structures will change from the traditional organization by function to a highly centralized management with few levels, small staffs, and hands-on control by managers with high-capacity personal computers networking with massive databases.

Another gloomy picture was offered by William Johnson, president of Jofree Corp. and former chief economist with Tenneco Inc. Most of the oil industry's problems Johnson traces to OPEC's gyrations. He is skeptical about whether OPEC "can get its act together." Even if it does, he says, it probably will find that raising prices much above $20 per barrel would not benefit its long-term interests.

Some individuals and groups in the oil industry are saying that the U.S. is facing an inevitable national catastrophe. Currently, consumers are trading short-term price benefits for long-term security without even realizing that the trade is being made. Johnson questions that forecast, but he admits that there is reason for concern over future crises. The problem is the fear of shortages, and that, Johnson says, is the catalyst for another crisis.

Contrary to the opinion of many, Johnson maintains that U.S. supply security is still an issue. The Saudis are no longer functioning as the balance wheel in OPEC production. The Saudis are now in a full-scale oil price war with the other producers.

Johnson suggests that it may be wishful thinking to believe the U.S. is now in a better position to cope with another crisis. It is true that it is somewhat better insulated against politically inspired limitations on production or price increases. Natural gas access is better, and nuclear power is developing, if slower than many would like. Interfuel competition is greater than ever before and growing. However, it is not certain, he says, that these measures would safeguard the country from another "oil bumble."

It is not where the U.S. is but where it is going that should arouse concern, Johnson says. The decline in drilling activity is a severe problem. Current reserve additions are down to 30% for 1986, and domestic reserves won't support present production levels very long. The only option after current reserves are depleted will be more imports, and the U.S. will be right back where it started in the 1970s.

With most attention being given to Middle East/European/North American oil problems, many observers fail to notice that future oil markets will be oriented increasingly in the Pacific. With the exception of Japan, Singapore, and Taiwan, most of the Pacific countries are developing, and the stakes for them are large indeed. Just how large was examined by Eugene D. McCarthy, division chief in the energy department at the World Bank. In the region are three significant oil-exporting countries—Indonesia, Malaysia, and China—and three significant oil-importing countries—South Korea, the Philippines, and Thailand. The exporters are expected to suffer from low prices and the importers to benefit. However, the simultaneous decline of the dollar will have adverse effects all around, with Japan probably affected most.

In contrast, OECD countries have been the chief beneficiaries of the price collapse, with Japan, West Germany, France, and Italy receiving about 40% of the total benefit. □